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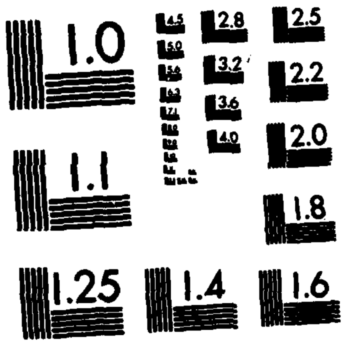

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Special Report for the period June 1981 to January 1982

Iterative Curve Fit of a Power Law Equation to Solid Propellant Shift Factor Data

November 1982

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FOREWORD

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number):

Software was developed for an HP-9815A programmable calculator which optimizes the constants of a single-valued algebraic or transcendental equation to fit a given set of experimental data. This technique was used to fit a power law equation to solid propellant shift factor vs temperature data. The results were compared to optimization methods suggested by the JANNAF Solid Propellant Structural Integrity Handbook and to the Power Law approximation reported in AFRPL-TR-81-66 for the same data.

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CONTENTS

LIST OF FIGURES

LIST OF SYMBOLS

a_T	time - temperature shift factor (dimensionless)
b	user specified number of cycles which iterative process is run
C_i	arbitrary unknown constant
E	sum of the squared errors
$\hat{E}$	root mean squared error
E(t)	relaxation modulus
m	positive exponent in power law a_T equation (dimensionless)
p	user specified multiple to generate search internal
T	temperature, degrees Fahrenheit (°F)
T_R	reference temperature, °F
T_a	constant in power law a_T equation, °F
T_g	glass transition temperature, °F
t	time, minutes (min)
α	constant in interval reducing function
β	constant in interval reducing function
ξ	reduced time

ITERATIVE CURVE FIT OF A POWER LAW EQUATION TO SOLID PROPELLANT SHIFT FACTOR DATA

1. INTRODUCTION

The JANNAF Solid Propellant Structural Integrity Handbook (Ref. 1) suggests an empirical power law relationship between temperature (T) and the time-temperature shift factor (a_T). To supplement existing solid propellant thermal transient viscoelastic response software (Ref. 2), an iterative method of fitting the transcendental equation relating T and a_T to a given set of experimental data was developed. This method was implemented in software formulated for use on a Hewlett-Packard 9815A programmable calculator (HP 9815A). It was decided that with minor changes the software could be modified to fit an arbitrary, single-valued, algebraic or transcendental equation to experimental data with the number of unknown constants limited only by the storage capacity of the calculator.

2. SUMMARY

The computer program developed for the HP 9815A successfully determines values for the unknown constants of the power law a_T equation in ten cycles or less, with a total run time of approximately ten minutes. These constants produce a curve which fits a given set of log a_T vs T data with less error than the trial and error method suggested by the JANNAF Solid Propellant Structural Integrity Handbook (Ref. 1). It also produced a better fit than the direct approximate solution suggested in AFRPL-TR-81-80 (Ref. 2).

This program was also expanded to fit a general function (either algebraic or transcendental, and having no more than three undetermined constants) to a given set of data. Due to lack of knowledge in making initial guesses for the constants, this curve fit does not converge as rapidly as the specific curve fit for the power law a_T equation. In fact, if the constants chosen produce too large an error, the iterative process will fail and new trial values must be selected. Modification of the storage capacity of this program would allow equations with more than three unknown constants to be evaluated.

3. SIGNIFICANCE OF A POWER LAW REPRESENTATION OF LOG (a_T) VS T PLOT

3.1 Definition of (a_T)

When a viscoelastic tensile test specimen is stretched (at a constant speed under uniform ambient temperature) to a specific strain level, the force required to maintain that strain level thereafter decreases with time. The modulus of elasticity will also be time dependent, and is denoted as the relaxation modulus E(t). This test is referred to as a relaxation test, and if it is performed at a series of ambient temperature levels, a group of similar shaped modulus curves plotted as log E(t) vs log time (t) may be obtained.

The assumption is now made that solid propellants are thermorheologically simple materials (Ref. 3) and that the time-temperature superposition principle is applicable. This implies that the group of curves generated from the relaxation tests are portions of a single master relaxation curve displaced (shifted along the log (t) axis due to the different temperature levels at which the tests were run.

The time-temperature shift factor (a_T) is defined as a non-dimensional measure of the shift in the log E(t) vs log (t) curve due to a change in the temperature of the relaxation test. Quantitatively, a_T is the distance along the log (t) axis between a value of log E(t) on a reference modulus curve and an equal value of log E(t) on the modulus curve for the temperature of interest. In practice, the relaxation modulus curves are treated as a single "master curve" of E(t) vs log ξ where ξ t/a_T is defined as the "reduced time" variable.

3.2 Power Law a_T Equation

An empirical power law equation has been developed (Ref. 2) to determine a value of a_T for a relaxation test run at a temperature above or below an arbitrary reference temperature (T_R) with the restriction that the temperature of interest must be greater than the glass transition temperature of the propellant. The relationship is as follows:

$$a_T = \left(\frac{T_R - T_a}{T - T_a}\right)^m \qquad (1)$$

T_a is a positive or negative constant with a suggested value of 10°F to 20°F below the glass transition temperature, and m is a positive constant (Ref. 2). The value of T_R *is usually in the range of 70°F to 80°F* (Ref. 2).

3.3 Application of the Power Law a_T Equation to Structural Analysis

The reduction of a thermal transient problem to an "ordinary linear viscoelastic" problem (Ref. 3) is based on the Moreland-Lee hypothesis used in conjunction with the previous assumption that the material is thermorheologically simple. *The Moreland-Lee hypothesis asserts that the reduced time under variable* temperature conditions is given by

$$\xi = \int_{\tau=0}^{\tau=t} \frac{d\tau}{a_T} \qquad (2)$$

The power law representation of $a_T(T)$ was developed to provide an analytically integrable function for the case of a linear temperature-time history and a restricted class of nonlinear temperature-time histories.

4. PROBLEM STATEMENT

From the preceding section, it becomes evident that the analyst needs a method to determine *the values of the arbitrary constants* T_a and m in the power law a_T equation in order to apply the Moreland-Lee hypothesis. Data relating a_T and T may be generated from a group of relaxation tests performed over a range of temperatures. The least squares method of fitting a curve to determine the values of the unknown constants results in a set of normal equations non-linear in the constants T_a and m. Therefore, a method is needed to generate the values of T_a and m for a_T vs T data such that the power law a_T equation fits this data with minimum error; i.e., to fit a transcendental equation with two or more unknown constants *to a given set of* data.

The term "error" will have two definitions in the following discussion. The root mean square error, $\hat{E}$, is defined as:

$$\hat{E} = \sum_{i=1}^{n} \frac{(\Delta Y_i)^2}{n} \tag{3}$$

where n is the number of data points and ΔY_i is the distance in the y direction between a data point (X_i, Y_i) and the point on the curve corresponding to X_i.

The sum of the squared errors, E, is defined as:

$$E = \sum_{i=1}^{n} (\Delta Y_i)^2 \tag{4}$$

5. SOLUTION

5.1 Assumptions

The following method of transcendental curve fitting was based on two assumptions:

(i) The n unknown constants C_i, i = 1...n produce an (n + 1) dimensional error surface which represents the error, E, in the curve fit due to a particular set of constants. When the intersection of level planes with this surface are projected into n-space, they are assumed to produce a group of inscribed contour lines (see Figure 1).

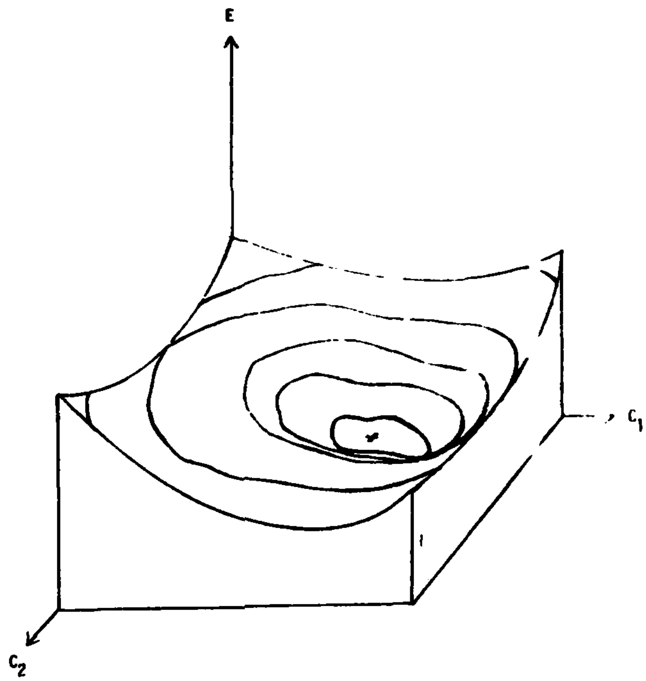

Figure 1. Hypothetical Error Surface, $E = f(C_i)$, for Two Unknown Constants.

(2) The function describing the error surface, $E = f(C_i)$, with respect to any constant C_i may be accurately approximated over a small interval by a quadratic equation, $f(C_i) = A(C_i)^2 + B(C_i) + D$, and a minimum value for this quadratic exists in the neighborhood of that small interval. The plots in Figures 2 and 3 are presented as examples of the curve representing $E = f(C_i)$ developed by fitting a quadratic through the three points marked "+." The points marked "o" are actual error points; it can be seen that over the interval used to develop the curve, the quadratic accurately approximates the actual error curve and that a minimum value exists in or near this interval.

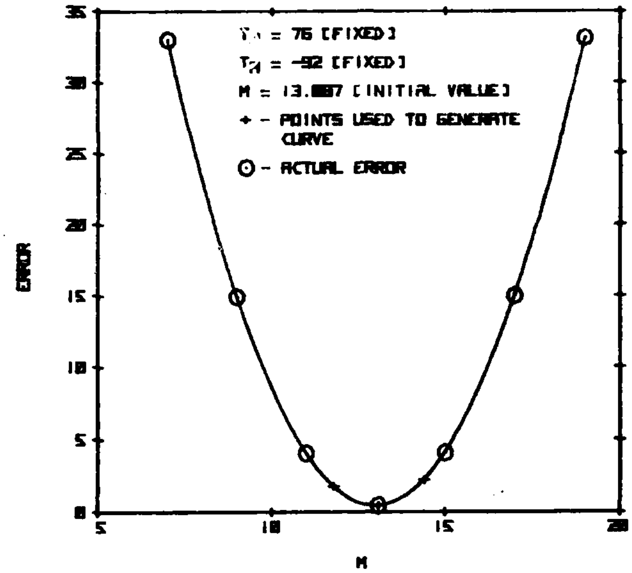

Figure 2. Variation of Error with m.

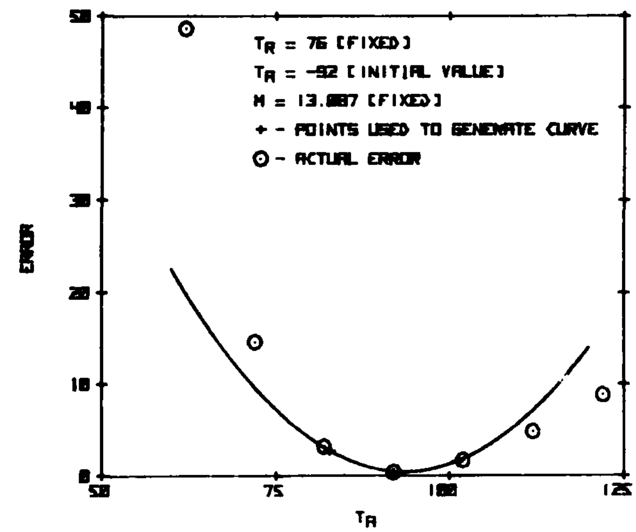

Figure 3. Variation of Error with T_a

The data for Figures 2 and 3 were generated from the log a_T vs T data used in the sample problem of Appendix A.

If the trial values of the constants are not relatively close to the values that minimize the error in the fit, the second assumption will not be valid. Also, Figure 3 shows that points on the actual error curve not in the immediate neighborhood of the points used to generate the quadratic are not necessarily well predicted by the quadratic.

5.2 Selection of Initial Trial Values

The curve fit technique developed is an iterative process that requires initial guesses at the unknown constants. The technique is very sensitive to these initial guesses. Therefore, a method was devised to develop initial guesses for T_a and m from a_T vs T data.

If a value of T_a equal to T_g is substituted into equation (1), a value of m may be determined from a least squares fit of the linear relationship (see Figure 4):

$$\log a_T = m \log \left(\frac{T_R - T_a}{T - T_a} \right) \tag{5}$$

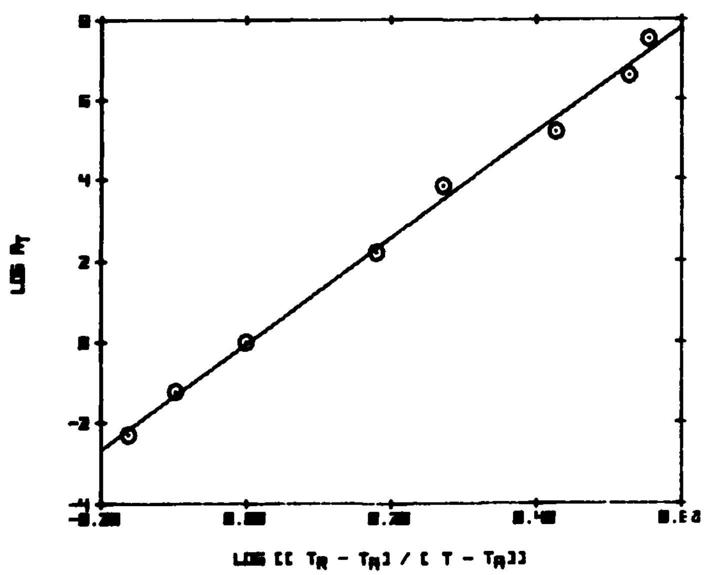

Figure 4. Least Squares Fit of Log a_T vs Log $\left[\frac{T_R - T_a}{T - T_a}\right]$ for sample problem in Appendix A.

A user knowing the values of T_R and T_g can thus obtain fairly accurate guesses at T_a and m. If T_R is unknown, a value between 70°F and 80°F should be used based on the definition of T_R in Section 3.2. If T_g is unknown, a trial and error procedure of guessing values for T_g and plotting

$$\log a_T = \log \left(\frac{T_R - T_a}{T - T_a} \right) \Bigg|_{T_a = T_g} \qquad (6)$$

should be used until a nearly straight line plot is obtained. The guess of T_g that yields this straight line plot should then be used as the initial guess for T_a.

The JANNAF Solid Propellant Structural Integrity Handbook (Ref. 1) suggests the above-described trial and error procedure to obtain the final a_T equation assuming a value of T_a 10°F to 20°F below T_g (Ref. 3). However, it was found in the present study that the best fits were obtained using the above method to generate guesses only and then iteratively operating on these guesses to obtain values that minimize the error of the fit.

5.3 Iterative Optimization of the Constants

The initial guesses of the unknown constants describe a point A (see Figure 5) in the T_a - m plane. The value of m is temporarily held constant, and points B and C are generated by adding and subtracting a user-specified multiple (p) of the present value of T_a to or from T_a, respectively. This search interval is labeled ΔT_a, and is equal to C_i = $p\, C_i$, where C_i equals T_a in Figure 5. In subsequent cycles, this search interval will be multiplied by a decreasing factor generated from the function

$$(1 - \beta) + \beta e^{(1-b)\alpha} \qquad (7)$$

where b is the number of the current iteration cycle, and α and β are user specified constants that determine the type (linear, exponential, etc.) and rate of interval reduction. This reduction in the search interval allows more accurate fits of a quadratic approximation to the error curve, producing a more accurate approximation of the minimizing value of C_i as the iterative process gets closer to the actual minimum values. In a more general sense, then, ΔC_i may be defined as

$$\Delta C_i = (p)(C_i)\left[(1-\beta) + \beta e^{(1-b)\alpha}\right] \qquad (8)$$

To assure that the quadratic approximation to the error has a minimum, the search interval will be expanded first in the negative C_i direction and then in the positive C_i direction until the values of E associated with the points B and C (E(B), E(C)) are greater than E(A). In the example shown, T_a is expanded in the negative T_a direction until the point $\overline{C}$ is located such that $E(\overline{C}) > E(A)$.

A quadratic is then fitted through $\overline{C}$, A, and B, and the first partial derivative, $\dfrac{\partial E(T_a, m)}{\partial T_a}$, is set equal to zero to find a new value of T_a (point D) which minimizes the error. See Appendix B for the methods used to fit the quadratic and take the partial derivative of the error.

Since the quadratic fit is only an approximation to the actual error function, a value of E corresponding to point D, E(D), is calculated and compared with the starting points E(A). If E(D) is greater than E(A), the new value T'_a will be rejected. If E(D) is less than or equal to E(A), the value T'_a will replace T_a as shown in Figure 5.

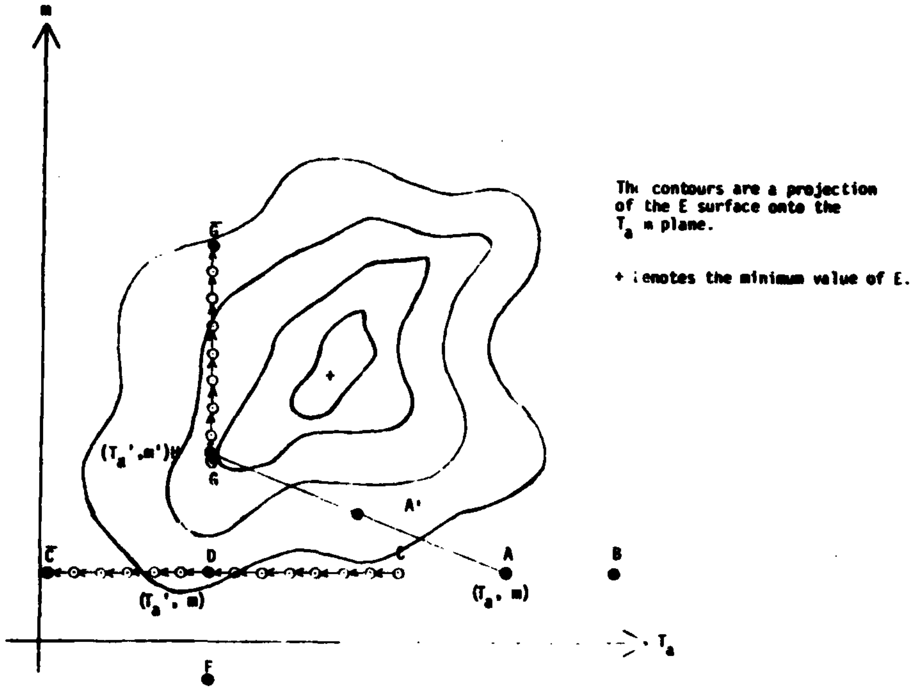

Figure 5. Iterative Optimization of the Constants, Cycle 1.

An identical process now operates on m (T_a temporarily fixed), with the quadratic fitted through points D, F, and G. A minimum value of the error is found at point H (T'_a, m'). The value of E corresponding to point H is compared to E(D), and the same acceptance criterion for this new point is applied. In Figure 6, E(H) was less than E(D).

One cycle of the procedure is now complete; and due to the comparisons, first of E(A) and E(D) and then E(H) and E(D), it is evident that the process has moved in the proper direction to reduce the error in the curve fit.

A likely starting point for the second cycle might be point H since it corresponds to the minimum E at present. However, to avoid the possibility of the process becoming "stuck" in a local valley of the error surface, a point A', midway between the newly calculated minimum point H and the starting point of that cycle

(point A), is determined and the process is started over (see Figure 6) at this intermediate point. The next cycle produces a new minimum at point H' and a new intermediate point A". Since the minimum value of E and the corresponding values of T_a and m are always stored in memory, these values can be (and are) selected on the final cycle rather than using the constants associated with A' for the final values.

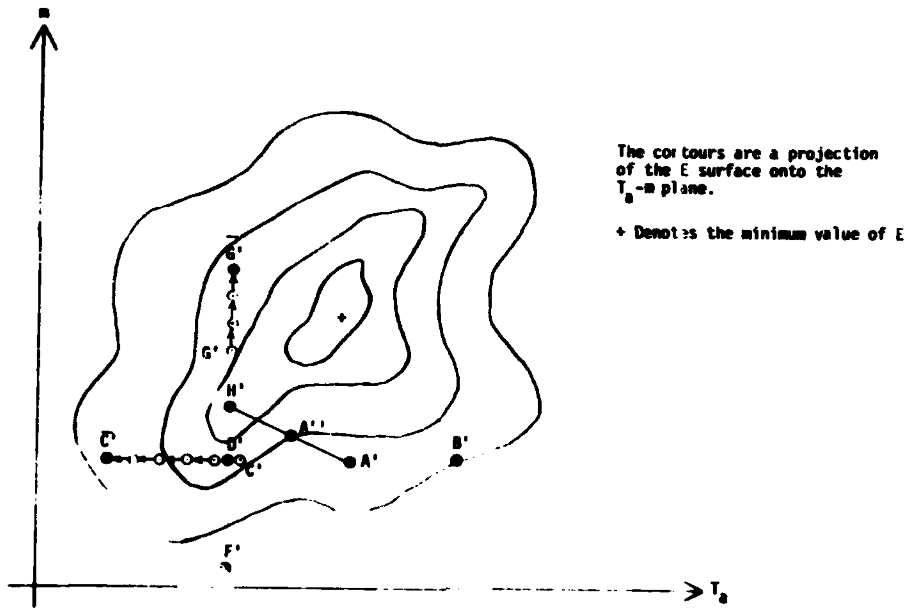

Figure 6. Iterative Optimization of the Constants, Cycle 2.

This process is repeated for a user-specified number of cycles or until the value of E at any point in the process becomes less than a user-specified minimum E.

It should be noted that T_R is considered a known constant, and the power-law a_T equation should ideally pass through the point (T_R, 0) on a log a_T vs T plot since

$$\log a_T \Big|_{T_R} = m \log\left(\frac{T_R - T_a}{T_R - T_a}\right) = 0 \qquad (9)$$

However, the log a_T vs T data will, most likely, have inherent error, and the curve which best fits this data may not necessarily pass through (T_R, 0), requiring the procedure to iterate on a third constant, T_R. Since both the assumptions of Section 5.1 hold for an n-dimensional problem, and since the equation for distance between two points may be extended to n dimensional space, this third constant presents no problem even though it produces a four dimensional error surface.

Appendix A illustrates a sample problem that uses this iterative process. Figure A-1 shows a plot of the curve generated by the iterative process along with the data used in the problem.

6. GENERAL CURVE FITTING

The method of optimizing the constants of a function described in Section 5 may be applied to any single-valued equation, either algebraic or transcendental. The problem again arises of picking initial values for the unknown constants. If arbitrary values are selected, the user must take care in choosing those values such that the equation of interest can be evaluated over a specified range when calculating the error. Also, the program must be modified to allow for the possible nonexistence of a minimum during any particular variable search.

Three modifications were made to the program previously developed to fit the power law α_T equation. First, the portion of the program that loads the data was modified to receive guesses rather than generate initial values from the data entered. Second, the user must program the equation of interest into the subroutine that calculates the sum of the squared errors. Third, the portion of the program that fits a quadratic through the error values and minimizes the function was modified to take into account the possibility that the curve has no minimum. If the curve is seeking a maximum, the program defaults to the one of three points used to determine the quadratic with the smallest E value and then proceeds to iterate on the next constant. If the curve is seeking a minimum outside the interval $(C_i - nC_i, C_i + nC_i)$, the interval over which C_i is expanded is doubled both in the plus and minus C_i direction until the minimum value of C_i lies within the interval of $(C_i - nC_i, C_i + nC_i)$ with the increased value of n.

Since arbitrary initial guesses are being used, the convergence of the general curve fit is not as rapid as the power law α_T fit. However, successive use of the program will allow a user to narrow down the choices for the constants and finally arrive at values that are accurate enough for assumption (2) of Section 5.1 to again be valid.

REFERENCES

1. JANNAF Solid Propellant Structural Integrity Handbook, Chemical Propulsion Information Agency (CPIA) Publication No. 230, September 1972.

2. Leighton, Russell A., "Quick Look Structural Analysis Techniques for Solid Rocket Propellant Grains," Air Force Rocket Propulsion Laboratory, Edwards Air Force Base, California. Report No. AFRPL-TR-81-80, May 1982.

3. Handbook for the Engineering Structural Analysis of Solid Propellants, Chemical Propulsion Information Agency (CPIA) Publication No. 214, May 1971.

APPENDIX A

SAMPLE PROBLEM

APPENDIX A. SAMPLE PROBLEM

This Appendix demonstrates a sample curve fit on the HP-9815A for the a_T vs T data tabulated at the end of the Appendix. Statements in quotations are user cues printed by the program. Numbers and words shown in boxes correspond to keystrokes needed to run the program.

I. Subroutine to Load Data

A. User enters the following to start the program:

[0] [Enter] [2] [Load] [Clear] [End] [R/S]

B. "PROGRAM TO LOAD DATA FOR A(T) VS T CUR\ E FIT"

"NO. OF DATA PTS?"

[8] [R/S]

(User enters the number of data points (up to twent··). If a number greater than twenty is entered, the message will be repeate l.)

C. "ENTER DATA (X,Y)"

Enter coordinates of data points (X is T in °F; Y is log a_T).

[-45] [R/S] (actual by stroke sequence is [4] [5] [CHS] [R/S])

"-45"

[7.52] [R/S]

"7.52"

•

•

•

[152] [R/S]

"152"

[-2.30] [R/S]

"-2.30"

D. "ENTER REF. TEMP. DEGREES F"

(If this value is unknown, see Section 5.2 for a range of values.)

[76] [R/S]

"76"

E. "ENTER GLASS TRANSITION TEMP., DEGREES F"

(This is used as an initial guess for T_a. If T_g is unknown, see Section 5.2 for a method of generating this value.)

$\boxed{-92}$ $\boxed{R/S}$

"-92"

A trial value of m is now computed by a least squares fit of log a_T vs log $(T_R - T_a)$ data, m being the slope of this line:

"m = 13.087"

F. "STORE ON TAPE?"

$\boxed{R/S}$ (For yes; $\boxed{\text{any numeric key}}$ then $\boxed{R/S}$ for no.)

This records the data points as well as the constants on tape.

G. "LOAD CURVE FIT?"

$\boxed{R/S}$ (For yes; $\boxed{\text{any numeric key}}$ then $\boxed{R/S}$ for no.)

This loads the subroutine that iteratively optimizes the constants.

II. Iterative Optimization of Constants

A. If this subroutine has not been loaded by the subroutine to load data, enter:

$\boxed{0}$ $\boxed{\text{enter}}$ $\boxed{7}$ $\boxed{\text{load}}$ $\boxed{\text{Clear}}$ $\boxed{\text{End}}$ $\boxed{R/S}$

(otherwise begin with Step B.)

B. "NO OF CONSTANTS 3 MAX"

Enter number of constants in the equation.

$\boxed{3}$ $\boxed{R/S}$

C. "ENTER SEARCH INTERVAL"

$\boxed{.10}$ $\boxed{R/S}$

(Since $a_T = m \log\left(\frac{T_R - T_a}{T - T_a}\right)$ must be evaluated at points generated by this constant (p), care must be taken in selecting this constant so the equation may be evaluated over the interval. In this problem, p is limited to .489. A value of p = .489 would cause the program to take the log of a negative number when iterating on T_a, producing an error condition. A value of 0.1 or smaller is recommended.)

D. "ENTER B"

[.9] [R/S]

E. "ENTER ALPHA"

[0.2] [R/S]

(These values, ALPHA and BETA (B), control the reduction of the interval with each cycle. B = .9, ALPHA = .2 give an exponential decay to a constant value.)

F. "ENTER TOLERANCE"

[0.02] [R/S]

(This value corresponds to a minimum E that the iterative process is trying to achieve. If this value is reached, the program will stop and print the constants associated with it.)

G. "NO OF ITERATIONS"

[10] [R/S]

(This corresponds to the number of cycles to be run. Convergence to three decimal places is usually achieved in 10 cycles or less with each cycle taking approximately 15 seconds if all three constants are iterated on.)

H. "SET FLAG I TO CONSTRAIN C_I"

[R/S]

Setting	Constrains
Flag 1	T_a
Flag 2	T_R
Flag 3	m

The best fit is obtained by leaving all three constants unconstrained. If T_R was to be constrained, the user would press [SFG] [2] [R/S]

I. "INITIAL VALUE OF CONSTANTS"

"92" (NOTE: The program assumes T_a is negative and only uses the magnitude of this number.)

[R/S]

"76"

R/S

"13.087"

R/S

SFG

Each constant is now redisplayed on the screen. If that constant is to be used, press R/S. If a different value is to be used, enter the value C_i and press R/S.

NOTE: When the final constant is printed, and R/S is hit, the SFG key should be hit immediately if the user wishes to have the error values printed out. Re-hitting SFG will stop the values from being printed.

J. Output and User Termination

The value of E for each cycle is printed, followed by the value of E after an iteration on one of the constants is performed, assuming SFG is pressed in Step I. The program will run the specified number of cycles unless E at any point becomes less than the tolerance, or the user terminates the program by pressing R/S Q. If the program runs its full number of cycles, the values of the final E and corresponding constants, as well as the minimum E and the corresponding constants, will be printed. If the user terminates the program at some intermediate point, the number of the current iteration cycle is printed along with current E and constants as well as minimum E and constants. Finally, if the tolerance is met, the value of E and constants which met or exceeded the tolerance will be printed. The number which flashes on the display indicates the current iteration cycle. Figure A-1 shows a plot of the data used for the problem and the curve fit obtained by the iterative method. The input data is also tabulated below.

Data used in sample problem

Log a_T	T (°F)
7.52	-45
6.60	-42
5.19	-29
3.84	-2
2.20	19
0.00	76
-1.23	118
-2.30	152

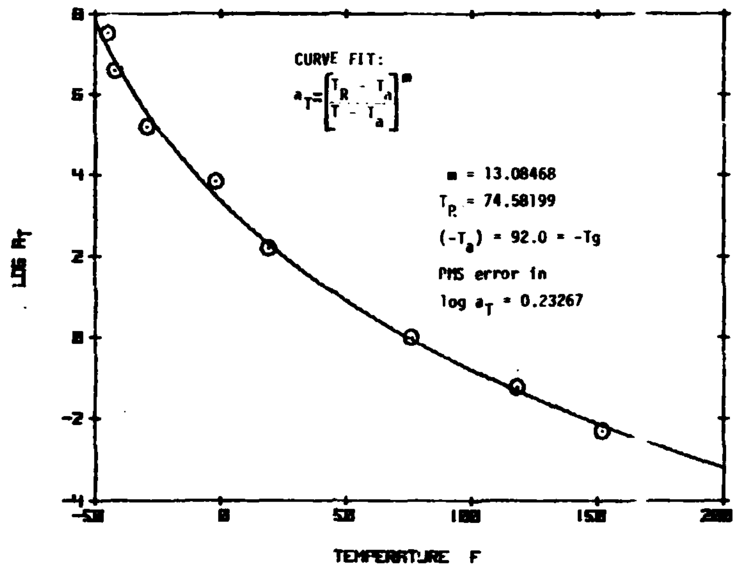

Figure A-1. Curve Fitted to Log a_T vs T Data

APPENDIX B

CURVE FIT AND MINIMIZATION OF ERROR

APPENDIX B. CURVE FIT AND MINIMIZATION OF ERROR

The following discussion outlines the procedure used to simultaneously fit a quadratic through the three points used to generate the error curve and find a value of C that minimizes this function (see Figure B-1). In this discussion, only one of the C_i's is considered to vary.

$$H = A(C_1)^2 + B(C_1) + D = E(C_1) \tag{B-1}$$

$$I = A(C_2)^2 + B(C_2) + D = E(C_2) \tag{B-2}$$

$$J = A(C_3)^2 + B(C_3) + D = E(C_3) \tag{B-3}$$

Simultaneous solution of equations (B-1) through (B-3) yields a quadratic fit of the squared error $E(C) = \Sigma\ (\Delta Y_i)^2$ through the three points.

$$A = \frac{C_1\ (J - I) + C_2\ (H - J) + C_3\ (I - H)}{C_1\ (C_3^2 - C_2^2) + C_2\ (C_1^2 - C_3^2) + C_3\ (C_2^2 - C_1^2)} \tag{B-4}$$

$$B = \frac{(I - J) - A(C_2^2 - C_3^2)}{(C_2 - C_3)} \tag{B-5}$$

The function $A(C_i)^2 + B(C_i) + D$ describes the squared error, $E(C_i)$. Taking the first partial derivative of E with respect to C_i and setting it equal to zero determines the minimum value of C_i

$$\frac{\partial E}{\partial C_i} = \frac{\partial (AC_i^2 + BC_i + D)}{\partial C_i} = 0$$

or

$$0 = 2AC_i + B$$

$$\text{and } C_{i\,min} = \frac{-B}{2A} \tag{B-6}$$

Direct substitution of equations (B-4) and (B-5) into equation (B-6) yields the value of C_i that minimizes the squared error E. Due to the location of the three points C_1, C_2, and C_3, the value computed in equation (B-6) is assured to be a minimum. See Section 5.3 for an explanation of the process of locating C_1, C_2, and C_3.

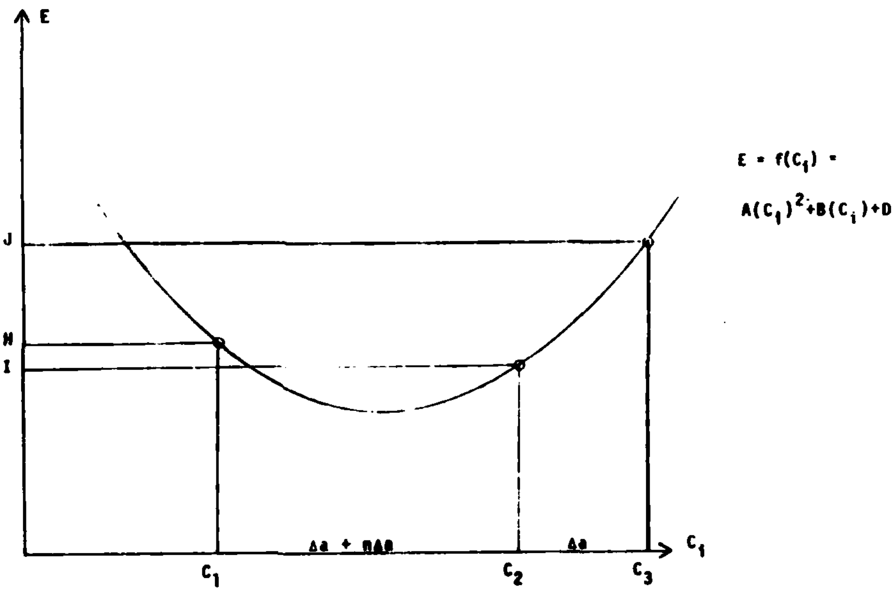

Figure B-1. Curve Fit and Minimization of $E = f(C_i)$

REFERENCES

1. JANNAF Solid Propellant Structural Integrity Handbook, Chemical Propulsion Information Agency (CPIA) Publication No. 230, September 1972.

2. Leighton, Russell A., "Quick Look Structural Analysis Techniques for Solid Rocket Propellant Grains," Air Force Rocket Propulsion Laboratory, Edwards Air Force Base, California. AFRPL-TR-81-80, May 1982.

3. Handbook for the Engineering Structural Analysis of Solid Propellants, Chemical Propulsion Information Agency (CPIA) Publication No. 214, May 1971.

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